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A method for constructing bicubic interpolation polynomials for the pressure P and internal energy E that are thermodynamically consistent at the mesh ponts and continuous across mesh boundaries is presented. The slope boundary conditions for the pressure and energy are derived from finite differences of the data and from Maxwell's consistency relation. Monotonicity of the sound speed and the specific heat is obtained by a bilinear interpolation of the slopes of the tabulated data. Monotonicity of the functions near steep gradients may be achieved by mesh refinement or by using a non-consistent bilinear fit to the data. Mesh refinement is very efficient for uniform-linear or uniform-logarithmic spaced data because a direct table lookup can be used. The direct method was compared to binary search and was 37 percent faster for logarithmic-spaced data and 106 percent faster for linear-spaced data. This improvement in speed is very important in the radiation-transport opacity-lookup part of the calculation. Interpolation in P-E space, with mesh refinement, can be made simple, robust, and conserve energy. In the final analysis the interpolation of the free energy and entropy (Maiden and Cook) remains a competitor.

Keywords: Equation of State, hydrodynamics, CFD, mix, radiation transport

I. Introduction

Current equation of state (EOS) tables at LLNL, (EOP), and LANL (SESAME) contain only internal energy $E(\rho, T)$ and pressure $P(\rho, T)$ as a function of temperature T and density ρ. They are fit with bilinear, bicubic, and rational polynomials. Bilinear methods are monotonic but the specific heat and sound speeds are discontinuous. Rational and cubic polynomials have undershoots near phase boundaries causing non-positive sound speeds and specific heats. The interpolants are not constrained to satisfy Maxwell's relations for thermodynamic consistency. Thermodynamic inconsistency may increase or decrease entropy thus causing an increase or decrease in temperature.

Maiden and Cook developed a thermodynamically consistent monotone bicubic interpolation of the Helmholtz free energy $F(\rho, T)$ or entropy $S(\rho, E)$. These functions are well behaved and discontinuities in the pressure appear as changes in slope of the potential function. The pressure and the energy are evaluated from derivatives of the interpolant. The method ensured thermodynamic consistency and is monotonic at the phase boundaries.

This paper presents a method for constructing bicubic interpolation functions of the pressure P(V,T) and internal energy E(V,T) that are thermodynamically consistent at the mesh points. The slope boundary condition of the bicubics are determined by finite differences of the tabulated data and from Maxwell's consistency condition. Because the interpolants may not be monotonic, the sound speed and specific heat at the mesh points are calculated from finite differences of the data and are bilinearly interpolated to maintain monotonicity. Corrections are made in the specific heat to conserve energy. In regions of sharp discontinuities local mesh refinement is prescribed to maintain accuracy and monotonicity. The refinement algorithm is based on hierarchical grids in which there is a nesting of uniform linear or logarithmic grids with refinement where it is needed near phase boundaries. The uniform grids permit direct table lookup which is faster than binary search. The methods described in this paper are simple, thermodynamically consistent, robust, and conserve energy.

II. Thermodynamic Consistency

Thermodynamic consistency requires that the thermodynamic data be derived from a potential function F(V,T). It also implies that the thermodynamic state F(V,T) is unique and independent of path, i.e., F is a state function of V and T. The derivatives F_V, F_T, F_{VT}, and F_{TV} are assumed to exist and be continuous. From the calculus Maxwell's relation is

$$F_{VT} = F_{TV}. \tag{1}$$

For the interpolant to be thermodynamically consistent it must satisfy this constraint and the thermodynamic variables must be defined as derivatives of the potential.

The first law of thermodynamics gives us the energy equation of the form

$$dE = -Pd\,V + dQ, \tag{2}$$

where $V = \rho^{-1}$ is the specific volume, and $dV = -\rho^2 d\rho$. The differential dQ is the heat release or gain per unit mass, and it may also be written as

$$dQ = TdS, \tag{3}$$

where S is the entropy, so that

$$dE = Td\,S - Pd\,V. \tag{4}$$

The Helmholtz free energy F(V,T) is defined as

$$F = E - TS\,. \tag{5}$$

Upon taking the differential and substituting Eqn. (4), we have

$$dF = -Pd\,V - SdT. \tag{6}$$

By taking the exact differential of F(V,T) and comparing terms, we find

$$S = -\left(\frac{\partial F}{\partial T}\right)_V \tag{7}$$

and

$$P = -\left(\frac{\partial F}{\partial V}\right)_T. \tag{8}$$

Differentiation of Eqns. (7) and (8) show that the pressure and the entropy must satisfy Maxwell's relation

$$\left(\frac{\partial P}{\partial T}\right)_V = \left(\frac{\partial S}{\partial V}\right)_T. \tag{9}$$

Currently, the EOP tables contain only pressure $P(\rho,T)$ internal energy $E(\rho,T)$. The entropy $S(\rho,T)$ is available for a limited number of materials. Upon taking the derivative $(\frac{\partial}{\partial V})_T$ of Eqn. (5) and subsituting Eqns. (8) and (9), we get the consistency condition

$$\left(\frac{\partial E}{\partial V}\right)_T = -P + T\left(\frac{\partial P}{\partial T}\right)_V. \tag{10}$$

This important equation expresses the dependence of internal energy on the volume at a fixed temperature solely in terms of measurables T, P, and V. It also means that the interpolants must satisfy this constraint.

III. Monotonicity

Thermodynamic stability requires that the isentropic sound speed C_S, isothermal sound speed C_T, and specific heat C_V be positive, i.e.,

$$C_T^2 = \left(\frac{\partial P}{\partial \rho}\right)_T > 0, \tag{11}$$

and

$$C_S^2 = \left(\frac{\partial P}{\partial \rho}\right)_S > 0, \tag{12}$$

The isentropic sound speed can be rewritten in terms of known quantities as

$$C_S^2 = \left(\frac{\partial P}{\partial \rho}\right)_T + \left(\frac{P}{\rho^2} - \left(\frac{\partial E}{\partial \rho}\right)_T\right)\frac{\left(\frac{\partial P}{\partial T}\right)_\rho}{\left(\frac{\partial E}{\partial T}\right)_\rho}. \tag{13}$$

When substituting the consistency condition Eqn. (10) into Eqn. (13) we get the sound speed with consistency

$$C_{SC}^2 = \left(\frac{\partial P}{\partial \rho}\right)_T + \frac{\frac{T}{\rho^2}\left(\frac{\partial P}{\partial T}\right)_\rho^2}{\left(\frac{\partial E}{\partial T}\right)_\rho}. \tag{14}$$

$$C_V = \left(\frac{\partial E}{\partial T}\right)_V > 0. \tag{15}$$

Also, many new numerical methods rely on Riemann solvers, and most of these methods require convexity of the EOS. That is,

$$\left(\frac{\partial^2 P}{\partial V^2}\right)_S > 0. \tag{16}$$

This condition may not be satisfied in regions of phase transitions and corrections to these hydrodynamic algorithms that have relied on convexity are neccessary.

IV. Approximate Thermodynamically Consistent Interpolation Scheme

The bicubic interpolation of free energy F and entropy S is currently the most effective method of interpolation of thermodynamic data (see Maiden and Cook). The scheme is consistent and has continuous first derivatives. Thermodyamically consistent interpolation schemes for the pressure P and energy E space can be derived but they are discontinuous at the mesh boundaries. In this paper a bicubic interpolation scheme is derived that is thermodynamically consistent only at the mesh points and continuous across mesh boundaries.

Bicubic: The bicubic interpolants are:

$$P = a_1 + b_1T + c_1V + d_1VT + e_1T^2 + f_1V^2 + g_1VT^2 + h_1V^2T + i_1V^2T^2$$
$$+j_1T^3 + k_1V^3 + l_1V^3T + m_1T^3V + n_1V^3T^2 + o_1T^3V^2 + p_1T^3V^3 \quad (17)$$
$$E = a_2 + b_2T + c_2v + d_2VT + e_2T^2 + f_2V^2 + g_2VT^2 + h_2V^2T + i_2V^2T^2$$
$$+j_2T^3 + k_2V^3 + l_2V^3T + m_2T^3V + n_2V^3T^2 + o_2T^3V^2 + p_2T^3V^3 \quad (18)$$

There are 32 constants to be determined by evaluating P and E and its first derivatives at the 4 mesh points. Evaluating the pressure P and energy E at the four mesh ponts determine 8 constants. Numerical differentiation of the tabulated data determine 12 slope boundary conditions and 8 twists. The remaining 4 slopes obtained from Maxwell's relation. There are 4 slopes related to the isothermal sound speeds and are given by

$$C_T^2 = -V^2\left(\frac{\partial P}{\partial V}\right)_T \quad (19)$$

There 4 slopes related to the specific heat and are given by

$$C_V = \left(\frac{\partial E}{\partial T}\right)_V \quad (20)$$

There are 4 slopes given by

$$\left(\frac{\partial P}{\partial T}\right)_V. \quad (21)$$

There are 8 twists given by

$$\left(\frac{\partial^2 E}{\partial V \partial T}\right)_{TV} \quad (22)$$

$$\left(\frac{\partial^2 P}{\partial V \partial T}\right)_{TV}. \quad (23)$$

Maxwells consistency condition Eqn. (10) gives us the remaing 4 slopes

$$\left(\frac{\partial E}{\partial V}\right)_T = -P + T\left(\frac{\partial P}{\partial T}\right)_V.$$

The pressure and energy are continuous, but there is no guarantee of monotonicity.

Bilinear: In the phase change regions of sharp discontinuity the bilinear interpolation may be appropriate. The bilinear functions of pressure $P(V,T)$ and internal energy $E(V,T)$ are given by

$$P = a_1 + b_1T + c_1V + d_1VT \quad (24)$$

$$E = a_2 + b_2 T + c_2 V + d_2 VT \tag{25}$$

The sound speed is given by

$$C_T^2 == V^2 \left(\frac{\partial P}{\partial V} \right)_T = -(c_1 + d_1 T) V^2 \tag{26}$$

The specific heat becomes

$$C_V = \left(\frac{\partial E}{\partial T} \right)_V = b_2 + d_2 V \tag{27}$$

V. Calculation of Sound Speed and Specific Heat

Significantly more accurate first derivatives (specific heat and sound speeds) can be obtained from the EOS tables by taking finite differences between three neighboring points $(x_{i=-1}, f_{i-1})$, (x_i, f_i), and (x_{i+1}, f_{i+1}) is given by at $x = x_i$ as

$$f'(x_i) = f_{i-1} \frac{(x_i - x_{i+1})}{(x_{i-1} - x_i)(x_{i-1} - x_{i+1})} + f_i \frac{(2x_i - x_{i-1} - x_{i+1})}{(x_i - x_{i-1})(x_i - x_{i+1})} + f_{i+1} \frac{x_i - x_{i-1}}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} \tag{28}$$

for equally spaced data $h = x_i - x_{i-1}$ the slope becomes the central difference formula

$$f'(x_i) = \frac{1}{2h} (f(x_{i+1}) - f(x_{i-1})) \tag{29}$$

In order to ensure monotonicity, the slopes of the EOS data are fitted with a bilinear interpolant as follows:

$$C_T = a_1 + b_1 T + c_1 \rho + d_1 \rho T \tag{30}$$

$$C_v = a_2 + b_2 T + c_2 \rho + d_2 \rho T \tag{31}$$

Energy Balance between mesh points T_0 and T_1 is

$$E_1 - E_0 = \int_{T_0}^{T_1} C_v dT \tag{32}$$

Where the specific heat at constant volume is given by

$$C_v = \left(\frac{\partial E}{\partial T} \right)_v \tag{33}$$

A linear variation of specific heat between mesh points is given by

$$C_v = \frac{C_{v1} - C_{v0}}{T_1 - T_0} (T - T_0) + C_{v0} + \epsilon \tag{34}$$

substituting linear expression for specific heat we get

$$E_1 - E_0 = (1/2)(C_{v1} + C_{v2})(T_1 - T_0) \quad (35)$$

where ϵ is an energy correction needed to maintain an energy balance. It is given by

$$\epsilon = E_1 - E_0 - (1/2)(C_{v0} + C_{v1})(T_1 - T_0) \quad (36)$$

is a small number and varies from zone to zone. The specific heat with energy balance correction is given by

$$\overline{C}_{v0} = C_{v0} + \epsilon \quad (37)$$

$$\overline{C}_{v1} = C_{v1} + \epsilon \quad (38)$$

The specific heat is discontinuous at the mesh ponts by a small amount ϵ.

VI. An Algorithm for Direct Table Lookup with Local Refinement

The EOP tables (P(ρ,T), and E(ρ,T) have unequal zoning in ρ and T space because refinement is required at phase boundaries. The EOP algorithm for locating the interpolation box for a given ρ, T pair is a binary search. Each zone in the hydrodynamics remembers which box it was in on the previous time cycle and used it as an initial guess for the next time cycle. The method is fast. However, in calculations in a region of phase change, the previous cycle guess may not be a good one.

The new idea in this paper is to apply local mesh refinement to resolve discontinuities at the phase boundary. The following describes the method. We define a multilevel mesh refinement algorithm for mesh generation of EOS data that will permit direct table lookup of EOS data needed in hydrodynamic codes. The method maps the ρ,T values to a set of integers. Linear and logarithmic functions are taken as examples. There is a savings of computer time over current search methods particularly in regions of a phase change where there are sharp discontinuities.

The idea is to map the mesh spacing into the integers for a direct table lookup. The location (i,j) of the interpolation box for given values of x and y is

$$(39) \qquad i(x) = int[f(x, x(0), n)]$$

$$(40) \qquad j(y) = int[f(y, y(0), m)]$$

where x(0) is the initial point corresponding i=0, n the number of zones, x is the horizontal location and y is the vertical location of the desired box. The space is coarsely divided with an evenly spaced mesh. Where the functional values have large variations such as phase boundaries the mesh is further locally refined with an evenly spaced mesh.

Uniform-linear-spaced data: Let a line be divided into n+1 equally spaced points containing n zones shown in Fig. 1. The distance between points is

$$dx = \frac{x(n) - x(0)}{n}. \quad (41)$$

The location of each node is

$$x(i) = x(0) + i * dx. \tag{42}$$

For any given x, the index of the left hand end point is given by

$$i(x) = int\left[(x(n) - x(1))/dx\right]. \tag{43}$$

In case local refinement is needed we can further subdivide into uniform sub grids.

Uniform Logarithmic spaced data: Similarly, we can subdivide logarithmically. Let a line be divided into n+1 equally spaced points containing n zones. Given x(0), x(n) and n then

$$x(i) = x(0)e^{i*dx} \tag{44}$$

At i=n we have

$$x(n) = x(0)e^{n*dx} \tag{45}$$

so the distance between points is

$$dx = \frac{1}{n}\log\left(\frac{x(n)}{x(0)}\right) \tag{46}$$

The location of each node is

$$x(i) = x(0)e^{i*dx} \tag{47}$$

For any given x, the index of the left hand end point is given by

$$i(x) = int\left[n\log\left(\frac{x}{x(0)}\right)\Big/dx\right] \tag{48}$$

For EOS data you may want to divide the temperature linearly and the density logarithmically. In the Helmholtz free energy $F(\rho,T)$ and the entropy $S(E,T)$ formulation the phase changes occur at changes in slope and only a coarse grid may be required.

Results: Figure 1. shows a comparison between binary search and the direct method for equally spaced logarithmic and linear data. The data shows that for equally spaced logarithmic zoning, Eqn. (48) is 37 percent faster and for equally spaced liner zoning, Eqn. (43) is 106 percent faster. This improvement in speed is very important in time-consuming weapons calculations, especially in the radiation-transport opacity-lookup part of the calculaton.

VII. Conclusion

In this paper a bicubic interpolation is derived for interpolating the pressure P and energy E. The scheme is thermodynamically consistent at the mesh ponts and continuous across mesh boundaries but there is no guarantee of monotonicity of the interpolant. Alternatively, in regions of a phase change a monotonic bilinear function could be used at the expense of consistency.

The sound speed and specific heat are calculated from the slopes of the tabulated data. This can be done very accurately using finite differences. Monotonicity of the sound speed and the specific heat can be guaranteed by bilinear fit of the slopes of the EOS surface. The specific heat at the mesh points can be adjusted to maintain energy conservation. This causes a slight discontinuity in the specific heat that is calculable.

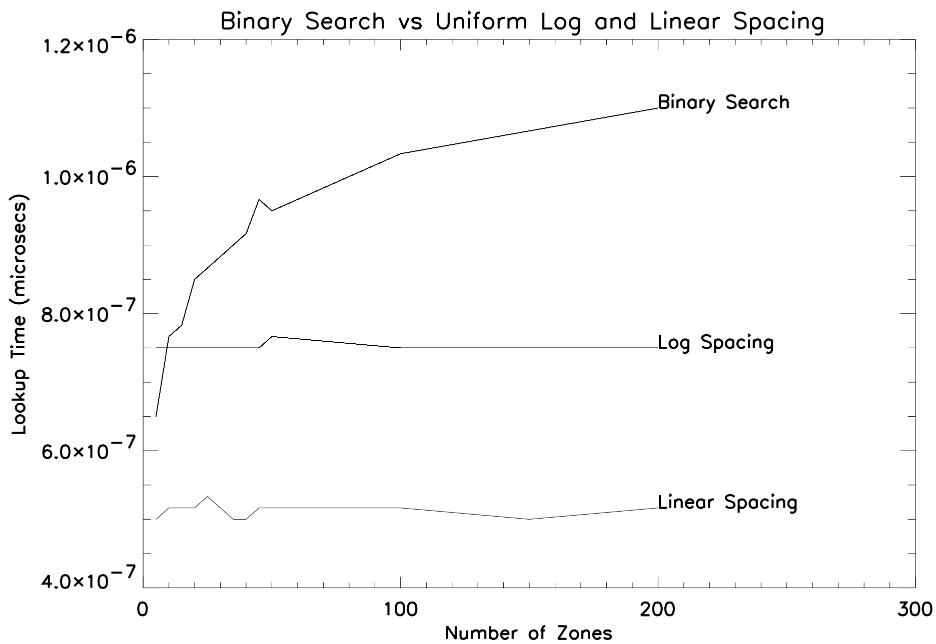

Figure 1: Comparison of lookup times between binary search, and direct lookup with uniform log spacing and linear spacing.

The bicubic fitting functions are very efficient and they can be made monotonic by local mesh refinement near steep gradients. Local mesh refinement causes no added expense because direct table lookup is used. It requires uniformly spaced linear or logarithmic data. Compared to binary search the direct method is 37 percent faster for logarithmic data and 106 percent faster for linear spaced data. The method speeds up the hydrodynamics but has a significant impact in opacity lookup in the radiation-transport part of the calculaton. The described methods are simple, robust, and conserve energy.

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